### **S&A FY03 Annual Review Meeting**

# On-Line Molecular Analysis for Improved Industrial Efficiency

R. W. Jones, J. J. Sweterlitsch, and J. F. McClelland Ames Laboratory – USDOE lowa State University

#### **Overview**

- Project Description: Real-time molecular analysis based on Transient Infrared Spectroscopy (TIRS)
- Objectives: Demonstrate TIRS on industrial processes in several IOF industries
- Overall goal: Increase industrial efficiency

### **Technical Merit/Need**

- Molecular processes are involved in 7 of the 10 IFOs including Agriculture, Mining, Petroleum, Forest Products, Chemical, Glass, and Supporting Industries
- Real-time, on-line molecular analyses can lead to improved efficiency in each of these industries

### Technical Merit/Need cont'd

- Molecular processes, from feedstock to finished products, can often be optimized if molecular composition is continuously sensed on-line and in realtime for automated process control.
- Currently, most molecular material analyses are done in the laboratory after production rather than during which does not serve process control needs.

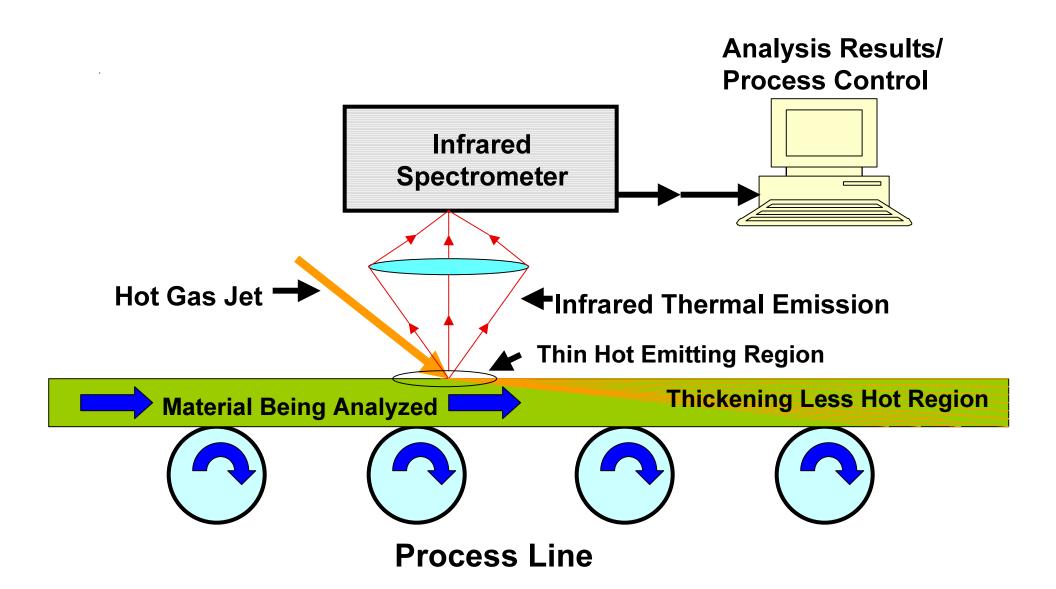
#### Technical Merit/Need cont'd

- Infrared molecular spectroscopy is widely used in industrial laboratories for molecular analysis.
- It is difficult to apply to on-line measurements using conventional methods due to their need for preanalysis sample preparation to reduce the opaqueness of most samples.

### **Technical Merit/Contribution**

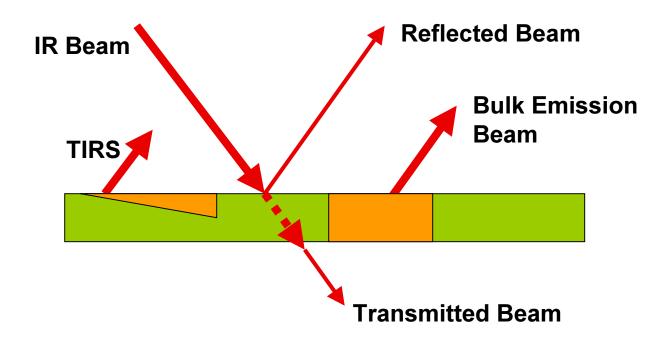
- Our innovation is to use the motion of the process line and the diffusion time of heat as it propagates into the sample to isolate in time a thin non-opaque layer of the sample for molecular analysis in real-time.
- This approach, called Transient Infrared Spectroscopy (TIRS), allows a thin-layer thermal emission spectrum of the material to be measured, which contains all of the molecular information provided by a conventionally measured infrared spectrum.

# **How Does TIRS Work?**

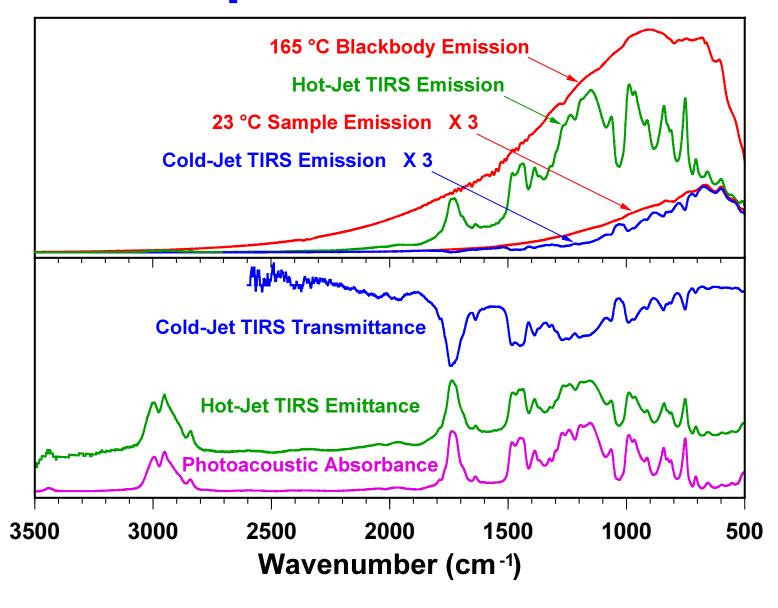


# How Does TIRS Compare to Conventional Methods

Transmission, reflection, and emission spectroscopies



## IR Spectra of PMMA



#### Where Can TIRS Be Used?

- On process lines that operate from high to low temperatures
- At line speeds from slow to very fast
- On processes running single fibers, irregular shaped flowing materials, viscous or nonviscous liquids, and nearly any sheet stock
- On process lines where noncontact remote sensing is desired

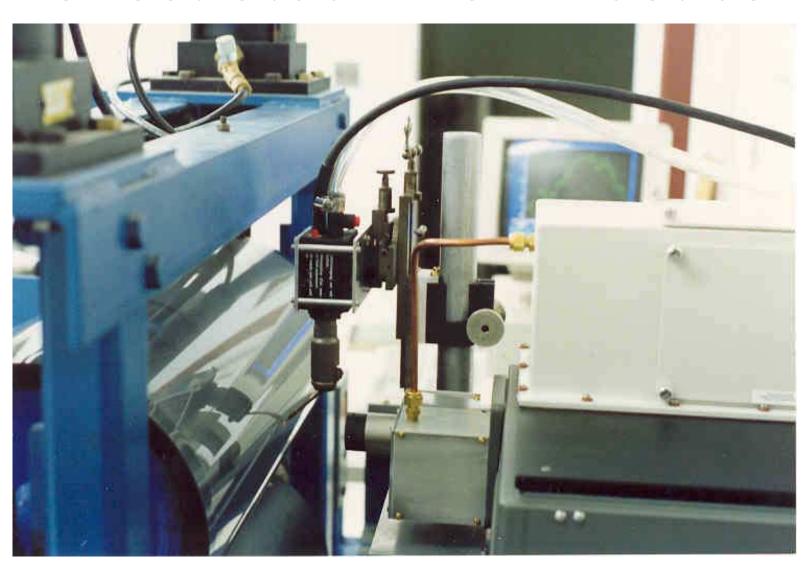
#### What Does TIRS Measure?

- Molecular composition of a wide range of materials
- Cure or polymerization of coatings
- Layer thicknesses of layered materials
- Copolymer, filler, and additive concentrations in engineering polymers
- Other material properties, such as mechanical, related to molecular composition

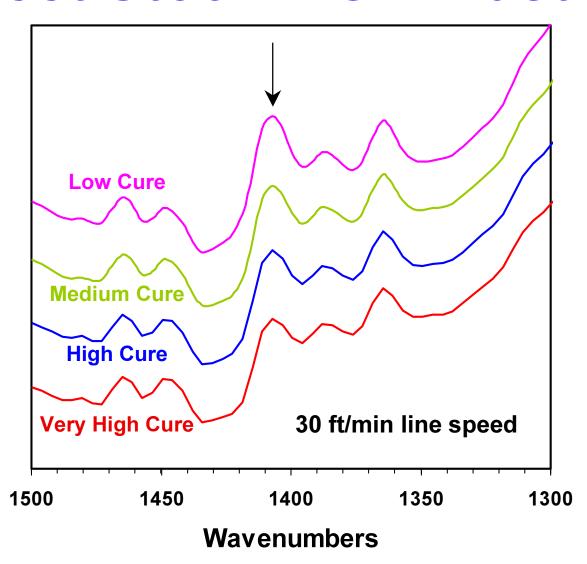
### **Examples of TIRS Applications**

- Monitoring cure of acrylic coating applied to plastic sheet stock (Petroleum and Chemicals Industries)
- Fiber-optic cladding and jacket cure monitor (Glass Industry)
- Wood chip chemical composition monitor (Forest Products Industry)

# Acrylic-Coating Cure on Plastic Sheet Stock – GE Plastics



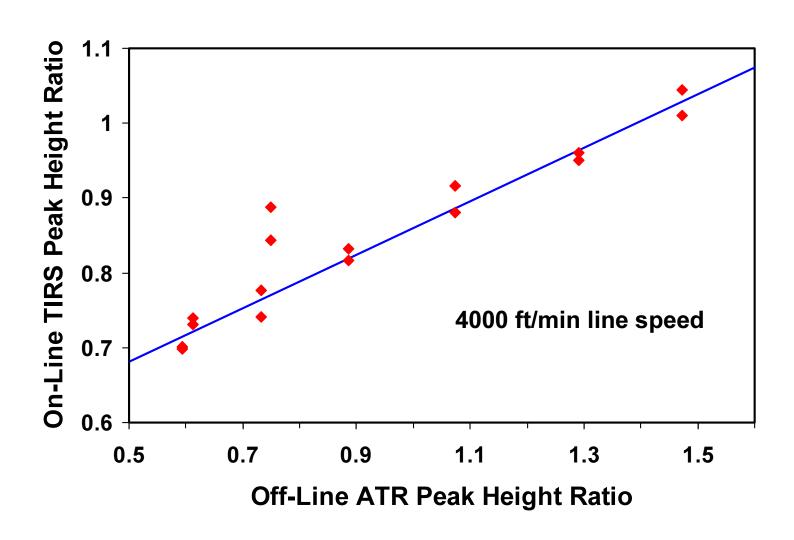
# Acrylic-Coating Cure on Plastic Sheet Stock – GE Plastics



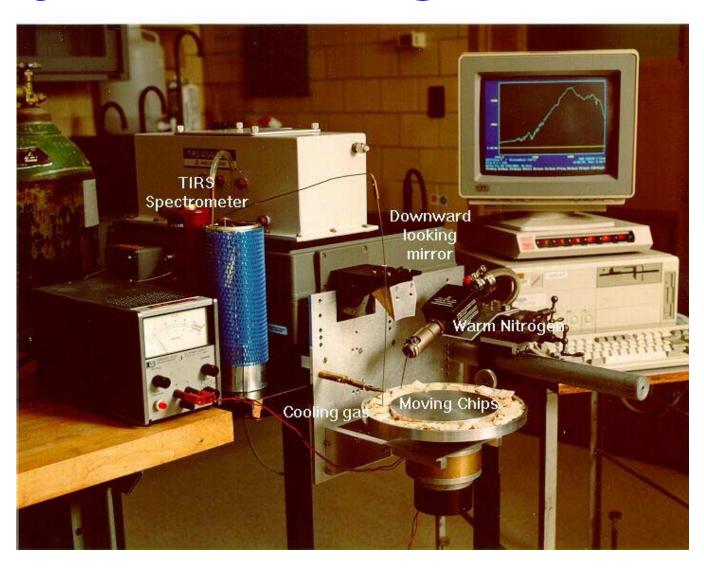
# Fiber-Optic Cable Jacket Cure - Corning



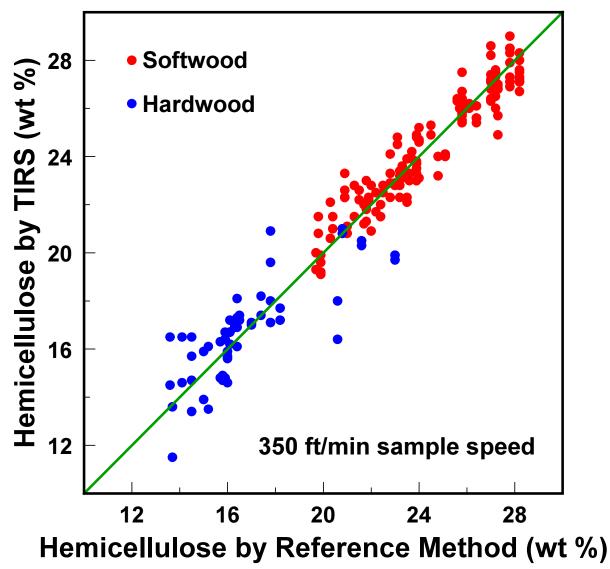
### Fiber-Optic Cladding Cure - Corning



# **Analysis of Moving Wood Chips**

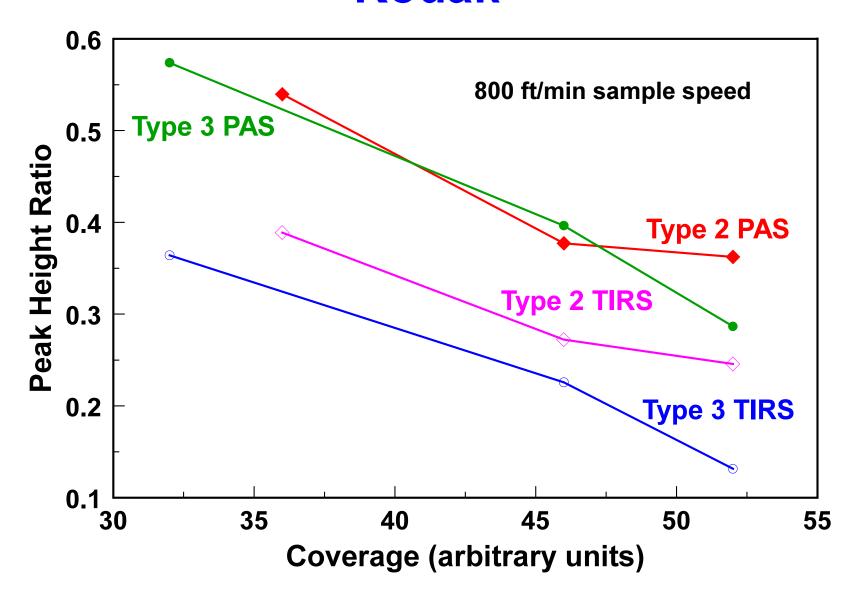


# **Hemicellulose of Wood Chips**



- Sensing thin-layer thicknesses on sheet stock – Kodak (Chemical)
- Monitoring cross-linking of biopolymers processed by reactive extrusion – Dept. of Food Science, Iowa State University (Agriculture)
- Monitoring the formulation engineering polymers at the extruder output – GE Plastics (Chemical and Petroleum)
- Detecting "sinker" wood in window frame manufacturing (unsuccessful) – Pella Window Corp. (Forest Products)

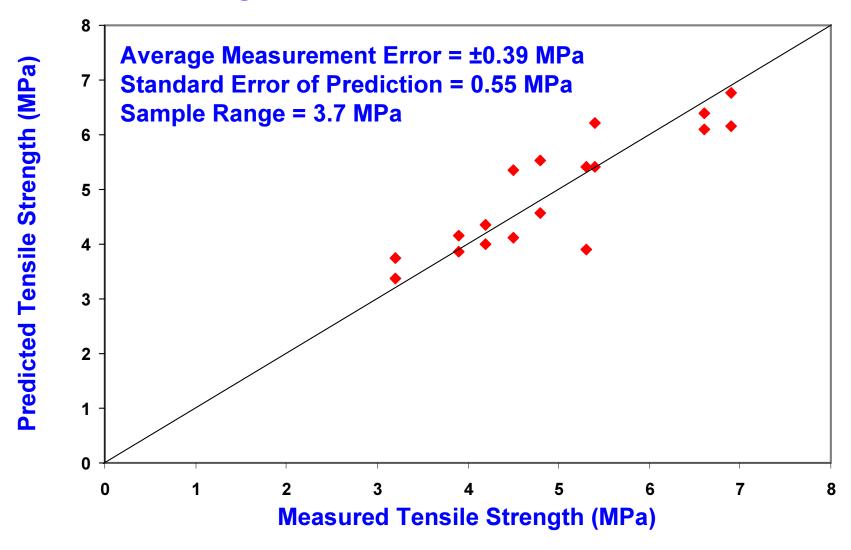
# Layer Coverage vs. TIRS Peak Ratio - Kodak



# **Cross-Linking of Biopolymers**



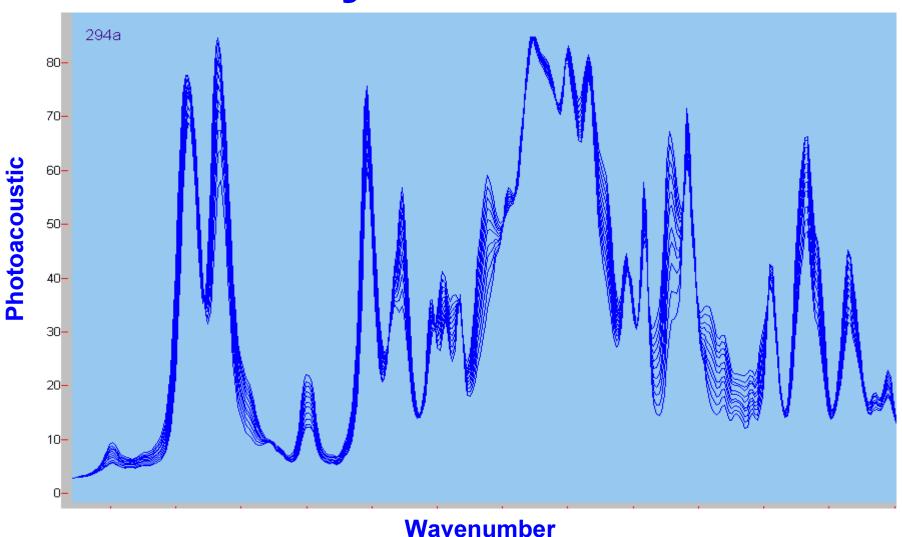
# Tensile Strength of Soy Plastics Containing Modified Rubber Additive



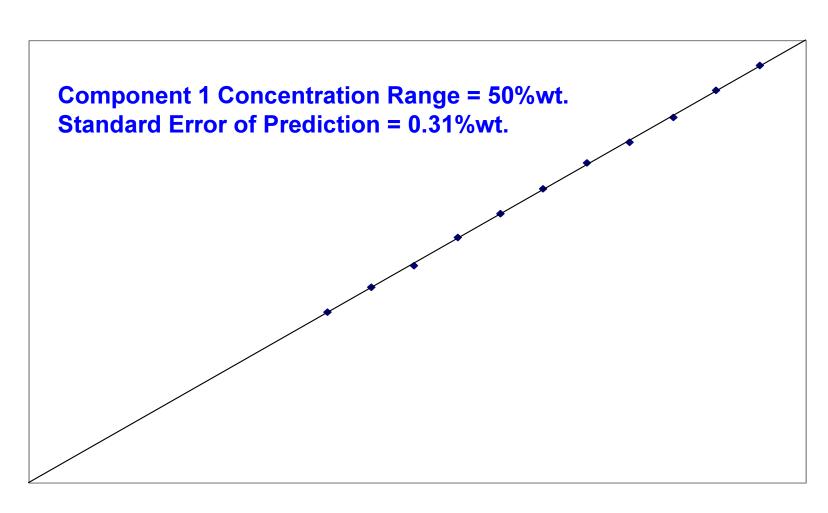
# PAS System for TIRS Feasibility Tests



# Photoacoustic Spectra of GE Polymer Blend

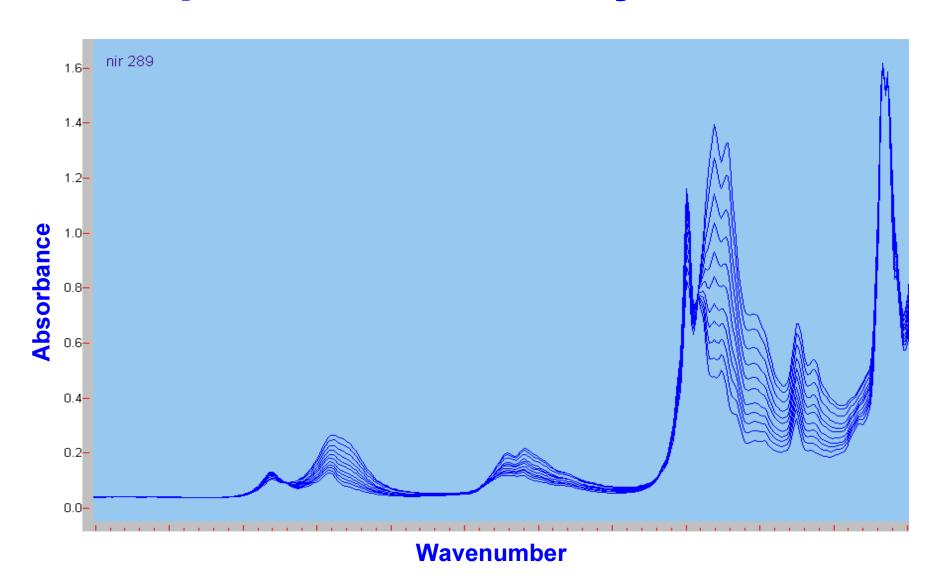


**Predicted Concentration Component 1** 

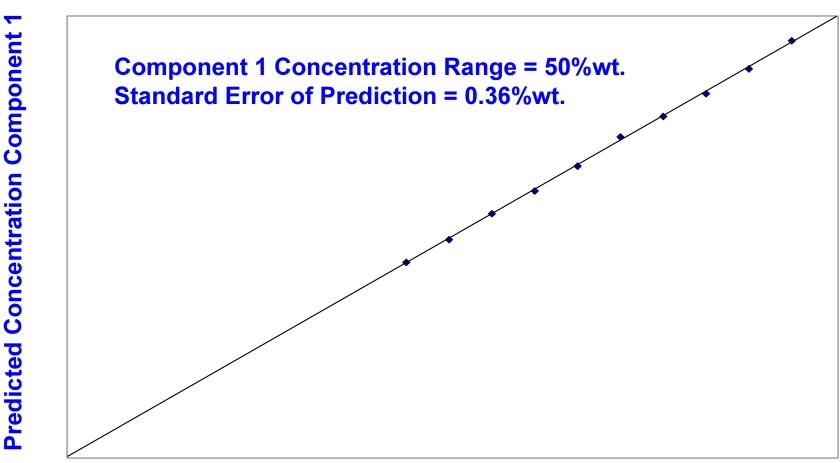


**Actual Concentration Component 1** 

# NIR Spectra of GE Polymer Blend



### **Prediction of Component 1 Concentration** for GE Polymer Blend from NIR Spectra



#### **Future Technical Milestones/Goals**

Milestone/Goal	<b>Expected date</b> of completion	Comments
Kodak site test/roll stock line	9-30-03	PAS & TIRS pretests done
GE/Mount Vernon site test/extruder line	9-30-03	PAS pretest in progress
GE/Selkirk site test/ extruder line	??	Need \$

#### **Possible Barriers:**

- Misperceptions of process engineers
- Continuity of funding

#### **Industrial End-User Involvement:**

- Kodak
- GE Plastics (Mount Vernon and Selkirk)
- Pella Window

Industrial involvement arranged through Pl's contacts in the research community

#### **Market Potential**

- Commercialization Plan:
   Partnership between ABB Bomem and
   MTEC Photoacoustics
- IOF Areas of Applicability:
   Agriculture, Mining, Petroleum, Forest Products, Chemical, and Supporting Industries are all molecular in nature
- What's Next:
  - Continue to demonstrate technology and to seek industrial installations

# **Programmatic Merit**

(In the case of polymers)

#### **Energy Benefits:**

Polymer processing consumes close to 1000 quads/year (Ashby,1992) so increases in efficiency can be significant

**Economic and Environmental Benefits:** 

Better control of polymer processing increases quality and reduces waste

M.F. Ashby, Materials Selection In Mechanical Design, Pergamon Press, 1992.

# **Summary**

- TIRS has the potential to increase general process efficiency and thus reduce energy and feedstock use, improve product quality, and reduce waste.
- TIRS is applicable to all of the "molecular" IOFs including agriculture, mining, petroleum, forest products, chemical, glass, and supporting industries.